STIC Search Report
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STIC Database Tracking Number: 162427

TO: Ben Sackey **Location: 5b31 / 5c18** **Art Unit: 1626** **Wednesday, August 31, 2005** **Case Serial Number: 10/690260**	**From: Noble Jarrell** **Location: Biotech-Chem Library** **Rem 1B71** **Phone: 272-2556** **Noble.jarrell@uspto.gov**

Search Notes

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16297

Noble

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: BEN SACKET Examiner #: 73489 Date: 8/12/05

Art Unit: 1626 Phone Number: 2- 0704 Serial Number: 10/690,260

Location (Bldg/Room#): 5B31 REM Mailbox #: 5C-18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Process for the racemate resolution of 3-Aminopentanenitrile

Inventors (please provide full names): Dreisbach et al.

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Process for obtaining enantiomerically enriched 3-aminopentanenitile or it's salt from racemic 3-aminopentanenitile comprising:

(1) reacting racemic 3-aminopentanenitile with an enantiomerically enriched organic acid

(2) Separating one diastereomeric salt from the reaction mixture and

(3) Converting the separated diastereomeric salt into the enantiomerically enriched 3-aminopentanenitile.

****

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Searcher: Noble

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 8/31/05

Searcher Prep & Review Time: 10

Online Time: 29

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

2 ✓ Structure (#)

✓ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

✓ STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____ In-house sequence systems

____ Commercial ____ Oligomer ____ Score/Length

____ Interference ____ SPDI ____ Encode/Transl

_____ Other (specify)

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=> d his

     (FILE 'HOME' ENTERED AT 09:26:12 ON 31 AUG 2005)

     FILE 'HCAPLUS' ENTERED AT 09:26:20 ON 31 AUG 2005
L1            1 US2004087811/PN OR (DE2002-10249339# OR US2003-690260#)/AP,PRN

     FILE 'REGISTRY' ENTERED AT 09:27:18 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 09:27:18 ON 31 AUG 2005
L2              TRA L1 1- RN :       51 TERMS

     FILE 'REGISTRY' ENTERED AT 09:27:18 ON 31 AUG 2005
L3           51 SEA L2

     FILE 'WPIX' ENTERED AT 09:27:21 ON 31 AUG 2005
L4            1 L1

=> b hcap;d all l1
FILE 'HCAPLUS' ENTERED AT 09:27:51 ON 31 AUG 2005
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FILE COVERS 1907 - 31 Aug 2005 VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L1 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:348005 HCAPLUS
DN 140:356956
ED Entered STN: 29 Apr 2004
TI Resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids.
IN Dreisbach, Claus; Schlummer, Bjoern
PA Bayer Chemicals AG, Germany
SO Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DT Patent
LA German
IC ICM C07B057-00
ICS C07C255-24
CC 23-19 (Aliphatic Compounds)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413565	A2	20040428	EP 2003-22897	20031009 <--
	EP 1413565	A3	20041013		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

DE 10249339	A1	20040513	DE 2002-10249339	20021022	<--
JP 2004143170	A2	20040520	JP 2003-359355	20031020	<--
US 2004087811	A1	20040506	US 2003-690260	20031021	<--
CN 1496971	A	20040519	CN 2003-10102878	20031022	<--

PRAI DE 2002-10249339 A 20021022 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
EP 1413565	ICM	C07B057-00	
	ICS	C07C255-24	
JP 2004143170	FTERM	4H006/AA02; 4H006/AC83; 4H006/AD15; 4H006/AD33; 4H006/BC51	<--
US 2004087811	NCL	558/463.000	<--

AB A process for obtention of enantiomerically enriched 3-aminopentanenitrile comprises treatment of racemic 3-aminopentanenitrile with an enantiomerically enriched organic acid to give 2 diastereomeric salts, separation of 1 of the salts from the reaction mixture, and conversion of the diastereomeric salt to enantiomerically enriched 3-aminopentanenitrile. Thus, reaction of racemic 3-aminopentanenitrile with (-)-diacetone-2-keto-L-gulonic acid in EtOH gave a precipitate which was recrystd. followed by dissoln. in 1N NaOH and extraction with CH2Cl2 to give (S)-3-aminopentanenitrile in 93.3% yield and 67.8% enantiomeric excess.

ST aminopentanenitrile resoln chiral org acid

IT Alcohols, uses
RL: NUU (Other use, unclassified); USES (Uses)
(C1-10; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Amino acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral, resolving agents; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Ethers, uses
RL: NUU (Other use, unclassified); USES (Uses)
(cyclic; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Carboxylic acids, uses
RL: NUU (Other use, unclassified); USES (Uses)
(esters; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(organic, chiral; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Resolution (separation)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Aromatic hydrocarbons, uses
Ethers, uses
Nitriles, uses
RL: NUU (Other use, unclassified); USES (Uses)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 400090-60-0P 639804-64-1P, (S)-3-Aminopentanenitrile
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 60-29-7, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 71-23-8, n-Propanol, uses 75-05-8, Acetonitrile, uses 108-88-3, Toluene, uses 109-99-9, Tetrahydrofuran, uses 141-78-6, Ethyl acetate, uses 1634-04-4, tert-Butyl methyl ether

RL: NUU (Other use, unclassified); USES (Uses)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 75-75-2, Methanesulfonic acid 7601-90-3, Perchloric acid, reactions 7647-01-0, Hydrochloric acid, reactions 7664-38-2, Phosphoric acid, reactions 7664-39-3, Hydrofluoric acid, reactions 7664-93-9, Sulfuric acid, reactions 7697-37-2, Nitric acid, reactions 10034-85-2, Hydriodic acid 10035-10-6, Hydrobromic acid, reactions 75405-06-0, 3-Aminopentanenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 79-33-4, L-Lactic acid, reactions 87-69-4, L-Tartaric acid, reactions 87-69-4D, L-Tartaric acid, derivs. 97-67-6, L-Malic acid 98-79-3 1188-21-2, N-Acetyl-L-leucine 2488-15-5, N-Boc-L-methionine 2592-18-9, N-Boc-L-threonine 2743-38-6, (-)-O,O'-Dibenzoyl-L-tartaric acid 3262-72-4, N-Boc-L-serine 3978-80-1, N-Boc-L-tyrosine 5104-49-4, 2-(2-Fluoro-4-biphenylyl)propionic acid 7536-55-2, N-Boc-L-asparagine 13139-15-6, N-(tert-Butoxycarbonyl)-L-leucine 13139-16-7, N-(tert-Butoxycarbonyl)-L-isoleucine 13734-34-4, N-Boc-L-phenylalanine 13734-41-3, N-Boc-L-valine 15761-38-3, N-Boc-L-alanine 15761-39-4, N-(tert-Butoxycarbonyl)-L-proline 17199-29-0, (S)-Mandelic acid 17791-52-5 18467-77-1 20246-53-1D, Gulonic acid, derivs. 22204-53-1 26164-26-1, (S)-Methoxyphenylacetic acid 40248-63-3, (-)-Menthoxyacetic acid 47358-42-9 51146-56-6, (S)-(+)-2-(4-Isobutylphenyl)propionic acid 102936-05-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agent; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 79-09-4D, Propionic acid, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agents; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

=> b wpix;d all l4
FILE 'WPIX' ENTERED AT 09:27:56 ON 31 AUG 2005
COPYRIGHT (C) 2005 THE THOMSON CORPORATION

FILE LAST UPDATED: 26 AUG 2005 <20050826/UP>
MOST RECENT DERWENT UPDATE: 200555 <200555/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://thomsonderwent.com/coverage/latestupdates/ <<<

>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER GUIDES, PLEASE VISIT:
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>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.
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FOR DETAILS. <<<
'BIX BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

L4 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-349508 [33] WPIX
DNC C2004-132937
TI Production of enantiomer enriched 3-aminopentanonitrile e.g. used as pharmaceutical intermediate, comprises reacting racemic 3-aminopentanonitrile with enantiomer enriched organic acid and separating diastereomeric salts.
DC B05
IN DREISBACH, C; SCHLUMMER, B
PA (FARB) BAYER AG; (FARB) BAYER CHEM AG; (DREI-I) DREISBACH C; (SCHL-I) SCHLUMMER B
CYC 35
PI EP 1413565 A2 20040428 (200433)* GE 11 C07B057-00
R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV MC MK NL PT RO SE SI SK TR
DE 10249339 A1 20040513 (200433) C07C255-24
US 2004087811 A1 20040506 (200433) C07C255-30 <--
JP 2004143170 A 20040520 (200434) 14 C07C253-32
CN 1496971 A 20040519 (200455) C07C055-24
KR 2004035568 A 20040429 (200456) C07C253-30
ADT EP 1413565 A2 EP 2003-22897 20031009; DE 10249339 A1 **DE 2002-10249339 20021022**; US 2004087811 A1 **US 2003-690260 20031021**; JP 2004143170 A JP 2003-359355 20031020; CN 1496971 A CN 2003-1102878 20031022; KR 2004035568 A KR 2003-73259 20031021
PRAI **DE 2002-10249339 20021022**
IC ICM C07B057-00; C07C055-24; C07C253-30; C07C253-32; C07C255-24; C07C255-30
ICS C07C253-30
AB EP 1413565 A UPAB: 20041125
NOVELTY - Production of enantiomer-enriched 3-aminopentanonitrile (APN) comprises reacting racemic APN with an enantiomer enriched organic acid to form two diastereomeric salts, separating one of the salts and converting it to enantiomer enriched APN or its salts.
USE - (R)-3-aminopentanonitrile is useful as a pharmaceutical intermediate.
ADVANTAGE - Products with a high enantiomeric excess (e.g. 60-80%) can be produced.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B10-A15

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FILE 'HOME' ENTERED AT 09:28:01 ON 31 AUG 2005

=>

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=> b reg;d ide l10 tot
FILE 'REGISTRY' ENTERED AT 09:42:45 ON 31 AUG 2005
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES:   30 AUG 2005  HIGHEST RN 862155-39-3
DICTIONARY FILE UPDATES:  30 AUG 2005  HIGHEST RN 862155-39-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html


L10  ANSWER 1 OF 9  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   853125-08-3  REGISTRY
ED   Entered STN:  28 Jun 2005
CN   Pentanenitrile-1-14C, 3-amino-, (3R)-, monomethanesulfonate (9CI)
     (CA INDEX NAME)
FS   STEREOSEARCH
MF   C5 H10 N2 . C H4 O3 S
SR   CA
LC   STN Files:   CA, CAPLUS

     CM   1

     CRN  853125-07-2
     CMF  C5 H10 N2

Absolute stereochemistry.
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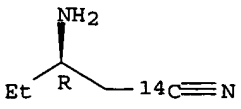


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     CM   2

     CRN  75-75-2
     CMF  C H4 O3 S
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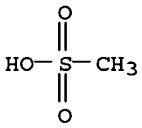
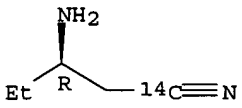


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **853125-07-2** REGISTRY
ED Entered STN: 28 Jun 2005
CN **Pentanenitrile-1-14C, 3-amino-, (3R)- (9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF **C5 H10 N2**
CI COM
SR CA

Absolute stereochemistry.

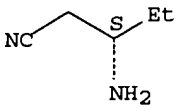


L10 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **688007-62-7** REGISTRY
ED Entered STN: 01 Jun 2004
CN **Pentanenitrile, 3-amino-, (3S)-, (2R,3R)-2,3-dihydroxybutanedioate (9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF **C5 H10 N2 . x C4 H6 O6**
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 639804-64-1
CMF C5 H10 N2

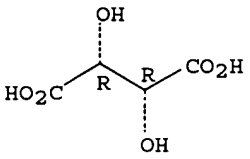
Absolute stereochemistry.



CM 2

CRN 87-69-4
CMF C4 H6 O6

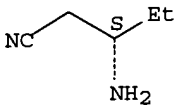
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **639804-64-1** REGISTRY
ED Entered STN: 21 Jan 2004
CN **Pentanenitrile, 3-amino-, (3S)- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **(S)-3-Aminopentanenitrile**
FS STEREOSEARCH
MF **C5 H10 N2**
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry.



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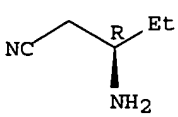
5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **474645-97-1** REGISTRY
ED Entered STN: 27 Nov 2002
CN **Pentanenitrile, 3-amino-, (3R)-, monomethanesulfonate (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **(R)-3-Aminopentanenitrile methanesulfonate salt**
CN **(R)-3-Aminopentanenitrile methanesulfonic acid salt**
FS STEREOSEARCH
MF **C5 H10 N2 . C H4 O3 S**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

CM 1

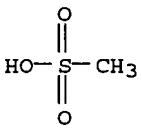
CRN 400090-60-0
CMF C5 H10 N2

Absolute stereochemistry.



CM 2

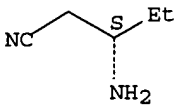
CRN 75-75-2
CMF C H4 O3 S



5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **400090-62-2** REGISTRY
ED Entered STN: 11 Mar 2002
CN **Pentanenitrile, 3-amino-, monohydrochloride, (3S)- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **(S)-3-Aminopentanenitrile hydrochloride**
FS STEREOSEARCH
MF **C5 H10 N2 . Cl H**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
CRN (639804-64-1)

Absolute stereochemistry.

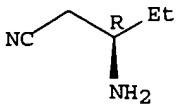


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **400090-61-1** REGISTRY
ED Entered STN: 11 Mar 2002
CN **Pentanenitrile, 3-amino-, monohydrochloride, (3R)- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **(R)-3-Aminopentanenitrile hydrochloride**
FS STEREOSEARCH
MF **C5 H10 N2 . Cl H**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
CRN (400090-60-0)

Absolute stereochemistry.

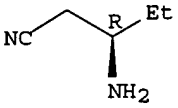


● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **400090-60-0** REGISTRY
ED Entered STN: 11 Mar 2002
CN **Pentanenitrile, 3-amino-, (3R)- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **(R)-3-Aminopentanenitrile**
FS STEREOSEARCH
MF **C5 H10 N2**
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPAT2, USPATFULL

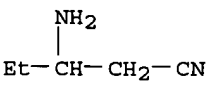
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **75405-06-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN **Pentanenitrile, 3-amino- (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **3-Aminopentanenitrile**
FS 3D CONCORD
MF **C5 H10 N2**
CI COM
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, CHEMLIST, PROMT, RTECS*, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)

Search done by Noble Jarrell

14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> => d his full

     (FILE 'HOME' ENTERED AT 09:26:12 ON 31 AUG 2005)

     FILE 'HCAPLUS' ENTERED AT 09:26:20 ON 31 AUG 2005
L1             1 SEA ABB=ON  PLU=ON  US2004087811/PN OR (DE2002-10249339# OR
                 US2003-690260#)/AP,PRN

     FILE 'REGISTRY' ENTERED AT 09:27:18 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 09:27:18 ON 31 AUG 2005
L2             TRA L1 1- RN :       51 TERMS

     FILE 'REGISTRY' ENTERED AT 09:27:18 ON 31 AUG 2005
L3            51 SEA ABB=ON  PLU=ON  L2

     FILE 'WPIX' ENTERED AT 09:27:21 ON 31 AUG 2005
L4             1 SEA ABB=ON  PLU=ON  US2004087811/PN OR (DE2002-10249339# OR
                 US2003-690260#)/AP,PRN

     FILE 'REGISTRY' ENTERED AT 09:36:49 ON 31 AUG 2005
L5             1 SEA ABB=ON  PLU=ON  639804-64-1 AND L3
L6           500 SEA ABB=ON  PLU=ON  C5H10N2
L7               QUE ABB=ON  PLU=ON  (PMS OR MAN OR IDS)/CI OR UNSPECIFED OR
                 COMPD OR COMPOUND OR (D OR T)/ELS
L8           402 SEA ABB=ON  PLU=ON  L6 NOT L7
L9            30 SEA ABB=ON  PLU=ON  L8 AND 3(1A)AMINO
L10            9 SEA ABB=ON  PLU=ON  (400090-60-0/BI OR 400090-61-1/BI OR
                 400090-62-2/BI OR 474645-97-1/BI OR 639804-64-1/BI OR 688007-62
                 -7/BI OR 75405-06-0/BI OR 853125-07-2/BI OR 853125-08-3/BI)
                 AND L9

     FILE 'HCAPLUS' ENTERED AT 09:43:36 ON 31 AUG 2005
L11           21 SEA ABB=ON  PLU=ON  L10
L12           24 SEA ABB=ON  PLU=ON  3(1A)(AMINOPENTANENITRILE OR AMINO(4A)(PENT
                 ANENITRILE OR PENTANE(1A)NITRILE))
L13           25 SEA ABB=ON  PLU=ON  (L11 OR L12)
L14            4 SEA ABB=ON  PLU=ON  L13(L) PUR/RL
                 E DREISBACH C/AU
L15           30 SEA ABB=ON  PLU=ON  ("DREISBACH C"/AU OR "DREISBACH CLAUS"/AU)
                 E SCHLUMMER B/AU
L16           13 SEA ABB=ON  PLU=ON  ("SCHLUMMER BJOERN"/AU OR "SCHLUMMER
                 BJORN"/AU)
L17        45851 SEA ABB=ON  PLU=ON  BAYER/CS,PA
L18            1 SEA ABB=ON  PLU=ON  L14 AND (L15 OR L16 OR L17)
L19            3 SEA ABB=ON  PLU=ON  L14 NOT L17

     FILE 'HCAOLD' ENTERED AT 09:48:57 ON 31 AUG 2005
L20            0 SEA ABB=ON  PLU=ON  (L11 OR L12)

     FILE 'USPATFULL, USPAT2' ENTERED AT 09:49:36 ON 31 AUG 2005
L21           17 SEA ABB=ON  PLU=ON  L11
                 E DRESISBACH C/AU
                 E DREISBACH C/AU
L22           23 SEA ABB=ON  PLU=ON  "DREISBACH CLAUS"/AU
                 E SCLUMMER B/AU
                 E SCHLUMMER B/AU
L23            3 SEA ABB=ON  PLU=ON  "SCHLUMMER BJORN"/AU
L24        14461 SEA ABB=ON  PLU=ON  L17
L25            1 SEA ABB=ON  PLU=ON  L21 AND (L22 OR L23 OR L24)
                 E RESOLUTION (SEPARATION)/CT
L26            4 SEA ABB=ON  PLU=ON  "RESOLUTION (SEPARATION)"/CT AND L21
L27            3 SEA ABB=ON  PLU=ON  L26 NOT L25
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     FILE 'WPIX' ENTERED AT 09:55:40 ON 31 AUG 2005
                 D DRN DCN L4
                 SEL DCN L4
L28          17 SEA ABB=ON  PLU=ON  (RA6AFL/SDCN OR RA7WAS/SDCN OR R00204/SDCN
                OR R00245/SDCN OR R00270/SDCN OR R00271/SDCN OR R00302/SDCN OR
                R00342/SDCN OR R00671/SDCN OR R00862/SDCN OR R00895/SDCN OR
                R01135/SDCN OR R01287/SDCN OR R01391/SDCN OR R01568/SDCN OR
                R10627/SDCN OR R19493/SDCN OR RAAVHB/SDCN)
L29           1 SEA ABB=ON  PLU=ON  L28 AND C5 H10 N2/MF
L30          18 SEA ABB=ON  PLU=ON  C5 H10 N2/MF
L31           3 SEA ABB=ON  PLU=ON  L30 AND (DCR-923913  OR DCR-738940 OR
                DCR-211181)/AN.S
                 SEL SDCN L31
L32          10 SEA ABB=ON  PLU=ON  (RAAVHB/DCN OR RAEPP0/DCN OR RA085P/DCN)
                E DREISBACH C/AU
L33          19 SEA ABB=ON  PLU=ON  "DREISBACH C"/AU
                E SCHLUMMER B/AU
L34           5 SEA ABB=ON  PLU=ON  "SCHLUMMER B"/AU
L35       30820 SEA ABB=ON  PLU=ON  BAYER/CS,PA
L36       30209 SEA ABB=ON  PLU=ON  FARB/PACO
L37           1 SEA ABB=ON  PLU=ON  L32 AND (L33 OR L34 OR L35 OR L36)
L38           9 SEA ABB=ON  PLU=ON  L32 NOT L37
L39      175186 SEA ABB=ON  PLU=ON  (B11-B OR C11-B OR E11-L OR E11-Q OR
                E11-Q01?)/MC OR N16?/M0,M1,M2,M3,M4,M5,M6 OR (C07C055 OR
                C07C057)/IPC
L40           1 SEA ABB=ON  PLU=ON  L38 AND L39
L41           9 SEA ABB=ON  PLU=ON  (L38 OR L40)

=> b hcap
FILE 'HCAPLUS' ENTERED AT 10:43:04 ON 31 AUG 2005
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FILE LAST UPDATED: 30 Aug 2005  (20050830/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d all fhitstr l18 tot

L18  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:348005  HCAPLUS
DN   140:356956
ED   Entered STN:  29 Apr 2004
TI   Resolution of 3-aminopentanenitrile using enantiomerically enriched
     organic acids.
IN   Dreisbach, Claus; Schlummer, Bjoern
PA   Bayer Chemicals AG, Germany
SO   Eur. Pat. Appl., 11 pp.
     CODEN: EPXXDW
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DT Patent
LA German
IC ICM C07B057-00
ICS C07C255-24
CC 23-19 (Aliphatic Compounds)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413565	A2	20040428	EP 2003-22897	20031009
	EP 1413565	A3	20041013		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10249339	A1	20040513	DE 2002-10249339	20021022
	JP 2004143170	A2	20040520	JP 2003-359355	20031020
	US 2004087811	A1	20040506	US 2003-690260	20031021
	CN 1496971	A	20040519	CN 2003-10102878	20031022
PRAI	DE 2002-10249339	A	20021022		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1413565	ICM	C07B057-00
	ICS	C07C255-24
JP 2004143170	FTERM	4H006/AA02; 4H006/AC83; 4H006/AD15; 4H006/AD33; 4H006/BC51
US 2004087811	NCL	558/463.000

AB A process for obtention of enantiomerically enriched 3-aminopentanenitrile comprises treatment of racemic 3-aminopentanenitrile with an enantiomerically enriched organic acid to give 2 diastereomeric salts, separation of 1 of the salts from the reaction mixture, and conversion of the diastereomeric salt to enantiomerically enriched 3-aminopentanenitrile. Thus, reaction of racemic 3-aminopentanenitrile with (-)-diacetone-2-keto-L-gulonic acid in EtOH gave a precipitate which was recrystd. followed by dissoln. in 1N NaOH and extraction with CH2Cl2 to give (S)-3-aminopentanenitrile in 93.3% yield and 67.8% enantiomeric excess.

ST aminopentanenitrile resoln chiral org acid

IT Alcohols, uses
RL: NUU (Other use, unclassified); USES (Uses)
(C1-10; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Amino acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral, resolving agents; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Ethers, uses
RL: NUU (Other use, unclassified); USES (Uses)
(cyclic; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Carboxylic acids, uses
RL: NUU (Other use, unclassified); USES (Uses)
(esters; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(organic, chiral; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Resolution (separation)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT Aromatic hydrocarbons, uses
Ethers, uses
Nitriles, uses
RL: NUU (Other use, unclassified); USES (Uses)

(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT **400090-60-0P 639804-64-1P**, (S)-3-**Aminopentanenitrile**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(resolution of **3-aminopentanenitrile** using enantiomerically enriched organic acids)

IT 60-29-7, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 71-23-8, n-Propanol, uses 75-05-8, Acetonitrile, uses 108-88-3, Toluene, uses 109-99-9, Tetrahydrofuran, uses 141-78-6, Ethyl acetate, uses 1634-04-4, tert-Butyl methyl ether
RL: NUU (Other use, unclassified); USES (Uses)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 75-75-2, Methanesulfonic acid 7601-90-3, Perchloric acid, reactions 7647-01-0, Hydrochloric acid, reactions 7664-38-2, Phosphoric acid, reactions 7664-39-3, Hydrofluoric acid, reactions 7664-93-9, Sulfuric acid, reactions 7697-37-2, Nitric acid, reactions 10034-85-2, Hydriodic acid 10035-10-6, Hydrobromic acid, reactions 75405-06-0, 3-Aminopentanenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

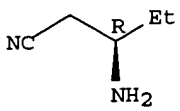
IT 79-33-4, L-Lactic acid, reactions 87-69-4, L-Tartaric acid, reactions 87-69-4D, L-Tartaric acid, derivs. 97-67-6, L-Malic acid 98-79-3 1188-21-2, N-Acetyl-L-leucine 2488-15-5, N-Boc-L-methionine 2592-18-9, N-Boc-L-threonine 2743-38-6, (-)-O,O'-Dibenzoyl-L-tartaric acid 3262-72-4, N-Boc-L-serine 3978-80-1, N-Boc-L-tyrosine 5104-49-4, 2-(2-Fluoro-4-biphenylyl)propionic acid 7536-55-2, N-Boc-L-asparagine 13139-15-6, N-(tert-Butoxycarbonyl)-L-leucine 13139-16-7, N-(tert-Butoxycarbonyl)-L-isoleucine 13734-34-4, N-Boc-L-phenylalanine 13734-41-3, N-Boc-L-valine 15761-38-3, N-Boc-L-alanine 15761-39-4, N-(tert-Butoxycarbonyl)-L-proline 17199-29-0, (S)-Mandelic acid 17791-52-5 18467-77-1 20246-53-1D, Gulonic acid, derivs. 22204-53-1 26164-26-1, (S)-Methoxyphenylacetic acid 40248-63-3, (-)-Menthoxyacetic acid 47358-42-9 51146-56-6, (S)-(+)-2-(4-Isobutylphenyl)propionic acid 102936-05-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agent; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT 79-09-4D, Propionic acid, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolving agents; resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

IT **400090-60-0P**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(resolution of **3-aminopentanenitrile** using enantiomerically enriched organic acids)

RN 400090-60-0 HCAPLUS
CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d all hitstr l19 tot

L19 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:513157 HCAPLUS
DN 141:70362
ED Entered STN: 25 Jun 2004
TI Enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile
IN Allen, David R.; Mozhaev, Vadim V.; Valivety, Rao H.
PA USA
SO U.S. Pat. Appl. Publ., 12 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C12P013-00
INCL 435128000
CC 16-5 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7, 23
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004121435	A1	20040624	US 2002-327492	20021220
WO 2004058701	A2	20040715	WO 2003-US40508	20031219

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-327492 A 20021220
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004121435	ICM	C12P013-00
	INCL	435128000
US 2004121435	NCL	435/128.000
	ECLA	C12P013/00; C12P041/00D2
WO 2004058701	ECLA	C12P013/00; C12P041/00D2

OS CASREACT 141:70362
AB Methods for preparing enantiomerically enriched aminopentanenitriles are provided. The methods involve selective acylation of an enantiomeric mixture of 3-aminopentanenitrile or selective hydrolysis of an enantiomeric mixture of 3-aminopentanenitrile amide in the presence of an enzyme selected from the group comprising lipase, esterase, and acylase. The methods yield R-aminopentanenitrile, which can be used to produce pharmaceutical products.
ST enantiomerically enriched aminopentanenitrile enzymic prepn
IT Binary systems
(aqueous two-phase; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
IT pH
(biol. effect of; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
IT Enzymes, uses
RL: BCP (Biochemical process); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)
(com.; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
IT Temperature effects, biological
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
IT Resolution (separation)
(enzymic, kinetic; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
IT Hydrolysis

(enzymic, stereoselective; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT Acylation
Hydrolysis
(enzymic; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT Enzymes, uses
RL: BCP (Biochemical process); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)
(immobilized; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT Acylation
(stereoselective; enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 67-56-1, Methanol, processes 71-43-2, Benzene, processes 75-05-8, Acetonitrile, processes 75-09-2, Methylene chloride, processes 108-88-3, Toluene, processes 109-99-9, Tetrahydrofuran, processes 110-86-1, Pyridine, processes 123-91-1, 1,4-Dioxane, processes 1634-04-4, Methyl tert-butyl ether 7732-18-5, Water, processes
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 710339-75-6P 710339-76-7P 710339-77-8P 710339-78-9P
RL: BCP (Biochemical process); BMF (Bioindustrial manufacture); RCT (Reactant); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 9001-62-1, Chirazyme L-1 9014-06-6, Penicillin acylase 9016-18-6, Carboxyl esterase 9026-00-0, Cholesterol esterase
RL: BCP (Biochemical process); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 101-41-7, Methyl phenylacetate 103-81-1, Benzeneacetamide 103-82-2, Phenylacetic acid, reactions 123-20-6, Vinyl butyrate 123-86-4, Butyl acetate 141-78-6, Ethyl acetate, reactions 371-27-7 769-78-8, Vinyl benzoate 2065-23-8, Methyl phenoxyacetate 2146-71-6, Vinyl laurate 2743-38-6, Dibenzoyl-L-tartaric acid 3050-69-9, Vinyl caproate 75405-06-0, 3-Aminopentanenitrile 94808-70-5 177536-74-2 710339-74-5
RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 639804-66-3P
RL: BMF (Bioindustrial manufacture); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT **400090-60-0P**, R-3-**Aminopentanenitrile**
639804-64-1P, S-3-**Aminopentanenitrile**
RL: BMF (Bioindustrial manufacture); **PUR (Purification or recovery)**; BIOL (Biological study); PREP (Preparation)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

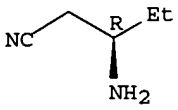
IT 75-75-2, Methanesulfonic acid 103-80-0, Phenylacetyl chloride
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT 474645-97-1P, R-3-Aminopentanenitrile methanesulfonate salt
RL: IMF (Industrial manufacture); PREP (Preparation)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

IT **400090-60-0P**, R-3-**Aminopentanenitrile**
639804-64-1P, S-3-**Aminopentanenitrile**

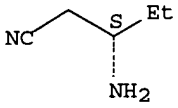
RL: BMF (Bioindustrial manufacture); **PUR (Purification or recovery)**; BIOL (Biological study); PREP (Preparation)
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)
RN 400090-60-0 HCAPLUS
CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639804-64-1 HCAPLUS
CN Pentanenitrile, 3-amino-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:409942 HCAPLUS
DN 140:391069
ED Entered STN: 20 May 2004
TI Preparation of optically active aminopentanenitrile
IN Morii, Seiji; Sato, Haruyo
PA Toray Industries, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07C253-34
ICS C07C255-24; C07B057-00; C07M007-00
CC 23-19 (Aliphatic Compounds)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2004143108	A2	20040520	JP 2002-311182	20021025
PRAI JP 2002-311182		20021025		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
JP 2004143108	ICM	C07C253-34
	ICS	C07C255-24; C07B057-00; C07M007-00
JP 2004143108	FTERM	4H006/AA02; 4H006/AC83; 4H006/AD15; 4H006/BB14; 4H006/BB31

OS MARPAT 140:391069
AB Title compound (I) is prepared by mixing racemic I with optically active carboxylic acids in solvents and crystallizing diastereomer salts. Racemic 3-I was mixed with N-benzenesulfonyl-L-phenylalanine in aqueous MeOH in the presence of HCl at 60° and cooled to 40° to give 54.1% diastereomer salt, which was treated with aqueous HCl, filtered, and the filtrate was treated with aqueous NaOH to give 50.1% (based on S-isomer in racemic I) (S)-3-I.
ST aminopentanenitrile optical resoln carboxylic acid diastereomer; phenylalanine benzenesulfonyl aminopentanenitrile optical resoln diastereomer
IT Amino acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(acidic; optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT Amino acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT Resolution (separation)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT Alcohols, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvents; optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT **400090-60-0P 639804-64-1P**, (S)-3-**Aminopentanenitrile**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT 688007-61-6P 688007-62-7P 688007-63-8P 688007-64-9P 688007-65-0P 688007-66-1P 688007-67-2P 688007-68-3P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

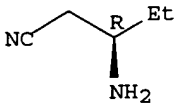
IT 87-69-4, L-Tartaric acid, reactions 1155-62-0, N-Benzyloxycarbonyl-L-glutamic acid 4816-80-2 13505-32-3 17447-35-7 20531-36-6, N-Benzenesulfonyl-L-glutamic acid 32634-68-7 40279-94-5 40279-95-6, N-Benzenesulfonyl-L-phenylalanine 75405-06-0, 3-Aminopentanenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT 67-56-1, Methanol, uses 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

IT **400090-60-0P 639804-64-1P**, (S)-3-**Aminopentanenitrile**
RL: IMF (Industrial manufacture); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(optical resolution of aminopentanenitrile by diastereomer salt formation with carboxylic acids)

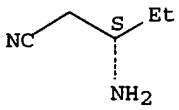
RN 400090-60-0 HCAPLUS
CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639804-64-1 HCAPLUS
CN Pentanenitrile, 3-amino-, (3S)- (9CI) (CA INDEX NAME)

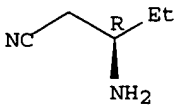
Absolute stereochemistry.



L19 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:924400 HCAPLUS
DN 136:196692
ED Entered STN: 23 Dec 2001
TI Isolation and structure determination of obyanamide, a novel cytotoxic cyclic depsipeptide from the marine cyanobacterium Lyngbya confervoides
AU Williams, Philip G.; Yoshida, Wesley Y.; Moore, Richard E.; Paul, Valerie J.
CS Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI, 96822, USA
SO Journal of Natural Products (2002), 65(1), 29-31
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
OS CASREACT 136:196692
AB Obyanamide was isolated from a variety of the marine cyanobacterium L. confervoides collected in Saipan, Commonwealth of the Northern Mariana Islands. Gross structure elucidation of this novel cyclic depsipeptide relied on extensive application of 2D NMR techniques. The absolute stereochem. was deduced by chiral chromatog. of the hydrolysis products and comparison with authentic and synthetic stds. Obyanamide was cytotoxic against KB cells with an IC50 of 0.58 μg/mL.
ST obyanamide cytotoxin cyclic depsipeptide Lyngbya
IT Toxins
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(cytotoxins; obyanamide, a novel cytotoxic cyclic depsipeptide from the marine cyanobacterium Lyngbya confervoides)
IT Peptides, biological studies
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(depsipeptides, cyclic; obyanamide, a novel cytotoxic cyclic depsipeptide from the marine cyanobacterium Lyngbya confervoides)
IT New natural products
(obyanamide (cyclic depsipeptide))
IT Lyngbya confervoides
(obyanamide, a novel cytotoxic cyclic depsipeptide from the marine cyanobacterium Lyngbya confervoides)
IT Molecular structure, natural product
(of obyanamide (cyclic depsipeptide))
IT 401818-00-6P, Obyanamide
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(obyanamide, a novel cytotoxic cyclic depsipeptide from the marine cyanobacterium Lyngbya confervoides)
IT 150736-71-3P, (R)-N-tert-Butyloxycarbonyl-2-aminobutanol 198493-28-6P, (R)-N-tert-Butyloxycarbonyl-3-aminopentane nitrile 400090-59-7P, (R)-N-tert-Butyloxycarbonyl-2-aminobutanol tosylate **400090-60-0P**, **(R)-3-Aminopentanenitrile**
RL: PRP (Properties); **PUR (Purification or recovery)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 3-aminopentanoic acid stds.)

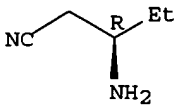
IT **400090-61-1P**, (R)-3-**Aminopentanenitrile** hydrochloride **400090-62-2P**, (S)-3-**Aminopentanenitrile** hydrochloride
RL: PRP (Properties); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 3-aminopentanoic acid stds.)
IT 5856-62-2, (S)-2-Aminobutanol 5856-63-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 3-aminopentanoic acid stds.)
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Carter, D; J Org Chem 1984, V49, P236 HCAPLUS
(2) Corbett, T; Cytotoxic Anticancer Drugs:Models and Concepts for Drug Discovery and Development 1992, P35
(3) Cragg, G; J Nat Prod 1997, V60, P52 HCAPLUS
(4) Golakoti, T; J Am Chem Soc 1995, V117, P12030 HCAPLUS
(5) Harrigan, G; J Nat Prod 1998, V61, P1221 HCAPLUS
(6) Klaus, R; Chromatographia 1989, V23, P137
(7) Kocienski, P; Protecting Groups 1994, P193
(8) Koehn, F; J Nat Prod 1992, V55, P613 HCAPLUS
(9) Luesch, H; J Nat Prod 2000, V63, P611 HCAPLUS
(10) Moore, R; Pure Appl Chem 1982, V54, P1919 HCAPLUS
(11) Ojika, M; Tetrahedron Lett 1995, V36, P5057 HCAPLUS
(12) Pettit, G; Heterocycles 1989, V28, P553 HCAPLUS
(13) Pettit, G; J Am Chem Soc 1982, V104, P905 HCAPLUS
(14) Pettit, G; J Nat Prod 1997, V60, P752 HCAPLUS
(15) Sone, H; Tetrahedron 1997, V53, P8149 HCAPLUS
(16) Sone, H; Tetrahedron Lett 1993, V34, P8449 HCAPLUS
(17) Sticher, O; J Nat Prod 2000, V63, P1283
(18) Tietze, L; Reactions and Synthesis in the Organic Chemistry Laboratory 1989, P437
(19) Trimurtulu, G; J Am Chem Soc 1994, V116, P4729 HCAPLUS
IT **400090-60-0P**, (R)-3-**Aminopentanenitrile**
RL: PRP (Properties); **PUR (Purification or recovery)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of 3-aminopentanoic acid stds.)
RN 400090-60-0 HCAPLUS
CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **400090-61-1P**, (R)-3-**Aminopentanenitrile** hydrochloride **400090-62-2P**, (S)-3-**Aminopentanenitrile** hydrochloride
RL: PRP (Properties); **PUR (Purification or recovery)**; SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 3-aminopentanoic acid stds.)
RN 400090-61-1 HCAPLUS
CN Pentanenitrile, 3-amino-, monohydrochloride, (3R)- (9CI) (CA INDEX NAME)

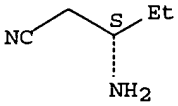
Absolute stereochemistry.



● HCl

RN 400090-62-2 HCAPLUS
CN Pentanenitrile, 3-amino-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

=> b uspatall
FILE 'USPATFULL' ENTERED AT 10:43:56 ON 31 AUG 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 10:43:56 ON 31 AUG 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

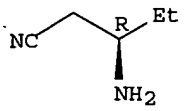
=> d bib abs fhitstr hitrn l25 tot

L25 ANSWER 1 OF 1 USPATFULL on STN
AN 2004:114964 USPATFULL
TI Process for the racemate resolution of 3-aminopentanenitrile
IN **Dreisbach, Claus**, Leichlingen, GERMANY, FEDERAL REPUBLIC OF
Schlummer, Bjorn, Leverkusen, GERMANY, FEDERAL REPUBLIC OF
PI US 2004087811 A1 20040506
AI US 2003-690260 A1 20031021 (10)
PRAI DE 2002-10249339 20021022
DT Utility
FS APPLICATION
LREP BAYER CHEMICALS CORPORATION, PATENT DEPARTMENT, 100 BAYER ROAD, PITTSBURGH, PA, 15205-9741
CLMN Number of Claims: 15
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 635
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB By means of a new process for the resolution of racemic 3-aminopentanenitrile, enantiomerically enriched 3-aminopentanenitrile or its salts can be obtained. For this, racemic 3-aminopentanenitrile is reacted with an enantiomerically enriched organic acid and one of the two diastereomeric salts formed is separated off and then converted into the enantiomerically enriched 3-aminopentanenitrile or its salts.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **400090-60-0P**
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic

acids)
RN 400090-60-0 USPATFULL
CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

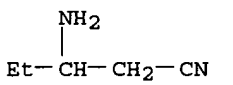


IT **400090-60-0P 639804-64-1P**, (S)-3-Aminopentanenitrile
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)
IT **75405-06-0**, 3-Aminopentanenitrile
(resolution of 3-aminopentanenitrile using enantiomerically enriched organic acids)

=> d bib abs hitstr l27 tot

L27 ANSWER 1 OF 3 USPATFULL on STN
AN 2005:44547 USPATFULL
TI Preparation of chiral amino-nitriles
IN Allen, David Robert, La Grange Park, IL, UNITED STATES
Achenbach-McCarthy, Crystal A., Lombard, IL, UNITED STATES
PI US 2005038281 A1 20050217
AI US 2004-946167 A1 20040921 (10)
RLI Continuation of Ser. No. US 2002-185092, filed on 28 Jun 2002, ABANDONED
DT Utility
FS APPLICATION
LREP BAKER & DANIELS, 300 NORTH MERIDIAN STREET, SUITE 2700, INDIANAPOLIS, IN, 46204-1782
CLMN Number of Claims: 31
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 545
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A process and intermediates for producing 3-amino nitrites. The process involves resolving an enantiomeric mixture of chiral 3-amino nitrites in the presence of a chiral acid in a solvent system to produce a chiral 3-amino nitrile salt. The process may further comprise a recrystalizing step, wherein an enantiomerically enriched 3-amino nitrile salt is produced. The process may further comprise a salt exchanging step, wherein another acid is added to the chiral 3-amino nitrile salt or the enantiomerically enriched 3-amino nitrile salt to produce another 3-amino nitrile salt.

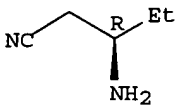
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **75405-06-0**, 3-Aminopentanenitrile
(resolution of 3-amino-nitriles by salt formation with acid enantiomers and purification by recrystn. and anion exchange of formed salt diastereomers)
RN 75405-06-0 USPATFULL
CN Pentanenitrile, 3-amino- (9CI) (CA INDEX NAME)



IT **400090-61-1P 474645-97-1P**
(resolution of 3-amino-nitriles by salt formation with acid enantiomers and purification by recrystn. and anion exchange of formed salt

diastereomers)
RN 400090-61-1 USPATFULL
CN Pentanenitrile, 3-amino-, monohydrochloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



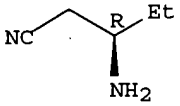
● HCl

RN 474645-97-1 USPATFULL
CN Pentanenitrile, 3-amino-, (3R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

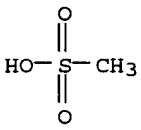
CRN 400090-60-0
CMF C5 H10 N2

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



L27 ANSWER 2 OF 3 USPATFULL on STN
AN 2004:158635 USPATFULL
TI Biocatalytic preparation of enantiomerically enriched aminopentanenitrile
IN Allen, David R., LaGrange Park, IL, UNITED STATES
Mozhaev, Vadim V., Hoffman Estates, IL, UNITED STATES
Valivety, Rao H., Schaumburg, IL, UNITED STATES
PI US 2004121435 A1 20040624
AI US 2002-327492 A1 20021220 (10)
DT Utility
FS APPLICATION
LREP BAKER & DANIELS, 300 NORTH MERIDIAN STREET, SUITE 2700, INDIANAPOLIS, IN, 46204-1782
CLMN Number of Claims: 56
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 967

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

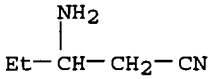
AB Methods for preparing enantiomerically enriched aminopentanenitriles are provided. The methods involve selective acylation of an enantiomeric mixture of 3-aminopentanenitrile or selective hydrolysis of an enantiomeric mixture of 3-aminopentanenitrile amide in the presence of an enzyme selected from the group comprising lipase, esterase, and acylase. The methods yield R-aminopentanenitrile, which can be used to produce pharmaceutical products.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **75405-06-0**, 3-Aminopentanenitrile
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

RN 75405-06-0 USPATFULL

CN Pentanenitrile, 3-amino- (9CI) (CA INDEX NAME)

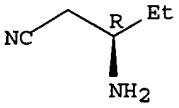


IT **400090-60-0P**, R-3-Aminopentanenitrile **639804-64-1P**, S-3-Aminopentanenitrile
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

RN 400090-60-0 USPATFULL

CN Pentanenitrile, 3-amino-, (3R)- (9CI) (CA INDEX NAME)

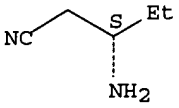
Absolute stereochemistry.



RN 639804-64-1 USPATFULL

CN Pentanenitrile, 3-amino-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **474645-97-1P**, R-3-Aminopentanenitrile methanesulfonate salt
(enzyme catalyzed preparation of enantiomerically enriched aminopentanenitrile)

RN 474645-97-1 USPATFULL

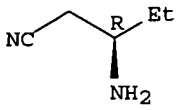
CN Pentanenitrile, 3-amino-, (3R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 400090-60-0

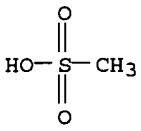
CMF C5 H10 N2

Absolute stereochemistry.



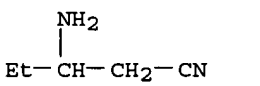
CM 2

CRN 75-75-2
CMF C H4 O3 S



L27 ANSWER 3 OF 3 USPATFULL on STN
AN 2004:2592 USPATFULL
TI PREPARATION OF CHIRAL AMINO-NITRILES
IN Allen, David Robert, La Grange Park, IL, UNITED STATES
Achenbach-McCarthy, Crystal A., Lombard, IL, UNITED STATES
PI US 2004002615 A1 20040101
AI US 2002-185092 A1 20020628 (10)
DT Utility
FS APPLICATION
LREP Kevin R. Erdman, Baker & Daniels, Suite 2700, 300 North Meridian Street, Indianapolis, IN, 46204
CLMN Number of Claims: 36
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 553
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A process and intermediates for producing 3-amino nitrites. The process involves resolving an enantiomeric mixture of chiral 3-amino nitrites in the presence of a chiral acid in a solvent system to produce a chiral 3-amino nitrile salt. The process may further comprise a recrystalizing step, wherein an enantiomerically enriched 3-amino nitrile salt is produced. The process may further comprise a salt exchanging step, wherein another acid is added to the chiral 3-amino nitrile salt or the enantiomerically enriched 3-amino nitrile salt to produce another 3-amino nitrile salt.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **75405-06-0**, 3-Aminopentanenitrile
(resolution of 3-amino-nitriles by salt formation with acid enantiomers and purification by recrystn. and anion exchange of formed salt diastereomers)
RN 75405-06-0 USPATFULL
CN Pentanenitrile, 3-amino- (9CI) (CA INDEX NAME)

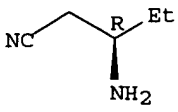


IT **400090-61-1P 474645-97-1P**
(resolution of 3-amino-nitriles by salt formation with acid enantiomers and purification by recrystn. and anion exchange of formed salt diastereomers)

Search done by Noble Jarrell

RN 400090-61-1 USPATFULL
CN Pentanenitrile, 3-amino-, monohydrochloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



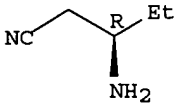
● HCl

RN 474645-97-1 USPATFULL
CN Pentanenitrile, 3-amino-, (3R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

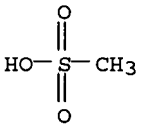
CRN 400090-60-0
CMF C5 H10 N2

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



=> b wpix
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=> d all l37 tot

L37  ANSWER 1 OF 1  WPIX  COPYRIGHT 2005 THE THOMSON CORP on STN
AN   2004-349508 [33]   WPIX
DNC  C2004-132937
TI   Production of enantiomer enriched 3-aminopentanonitrile e.g. used as
     pharmaceutical intermediate, comprises reacting racemic
     3-aminopentanonitrile with enantiomer enriched organic acid and separating
     diastereomeric salts.
DC   B05
IN   DREISBACH, C; SCHLUMMER, B
PA   (FARB) BAYER AG; (FARB) BAYER CHEM
     AG; (DREI-I) DREISBACH C; (SCHL-I) SCHLUMMER B
CYC  35
PI   EP 1413565      A2 20040428 (200433)* GE   11    C07B057-00
         R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV
            MC MK NL PT RO SE SI SK TR
     DE 10249339     A1 20040513 (200433)             C07C255-24
     US 2004087811   A1 20040506 (200433)             C07C255-30
     JP 2004143170   A  20040520 (200434)       14    C07C253-32
     CN 1496971      A  20040519 (200455)             C07C055-24
     KR 2004035568   A  20040429 (200456)             C07C253-30
ADT  EP 1413565 A2 EP 2003-22897 20031009; DE 10249339 A1 DE 2002-10249339
     20021022; US 2004087811 A1 US 2003-690260 20031021; JP 2004143170 A JP
     2003-359355 20031020; CN 1496971 A CN 2003-1102878 20031022; KR 2004035568
     A KR 2003-73259 20031021
PRAI DE 2002-10249339     20021022
IC   ICM  C07B057-00; C07C055-24; C07C253-30; C07C253-32; C07C255-24;
          C07C255-30
     ICS  C07C253-30
AB   EP   1413565 A UPAB: 20041125
     NOVELTY - Production of enantiomer-enriched 3-aminopentanonitrile (APN)
     comprises reacting racemic APN with an enantiomer enriched organic acid to
     form two diastereomeric salts, separating one of the salts and converting
     it to enantiomer enriched APN or its salts.
         USE - (R)-3-aminopentanonitrile is useful as a pharmaceutical
     intermediate.
          ADVANTAGE - Products with a high enantiomeric excess (e.g. 60-80%)
     can be produced.
     Dwg.0/0
FS   CPI
FA   AB; DCN
MC   CPI: B10-A15


=> d all l41 tot

L41  ANSWER 1 OF 9  WPIX  COPYRIGHT 2005 THE THOMSON CORP on STN
AN   2005-346647 [35]   WPIX
DNC  C2005-107199
TI   New racemic amino alkylnitrile compounds useful as building blocks in the
     synthesis of optically active beta-amino acids and pharmaceutical drugs.
DC   B05
```

IN COLBERG, J; FRANZ, S Z; MOTTERLE, R; STIVANELLO, M; COLBERG, J C; ZAMBELLI FRANZ, S
PA (PFIZ) PFIZER INC; (PFIZ) PFIZER PROD INC
CYC 108
PI WO 2005040097 A1 20050506 (200535)* EN 18 C07C253-32
RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW
US 2005107453 A1 20050519 (200535) A61K031-4172
ADT WO 2005040097 A1 WO 2004-IB3395 20041018; US 2005107453 A1 Provisional US 2003-515160P 20031028, US 2004-942985 20040917
PRAI US 2003-515160P 20031028; US 2004-942985 20040917
IC ICM A61K031-4172; C07C253-32
ICS A61K031-277; A61K031-401; A61K031-405; C07B057-00; C07C255-24; C07C255-29; C07D233-90
AB WO2005040097 A UPAB: 20050603
NOVELTY - Racemic amino alkylnitrile compounds (I) and their indivual R or S isomers are new.
DETAILED DESCRIPTION - Racemic amino alkylnitrile compounds of formula (I) and their indivual R or S isomers are new.
R = CH3, ethyl, n-propyl, isopropyl, n-butyl or isobutyl; and
A = N-acetyl-L-alanine, N-acetyl-L-arginine, N-acetyl-L-asparagine, N-acetyl-L-aspartic acid, N-acetyl-L-cysteine, N-acetyl-L-glutamine, N-acetyl-L-glutamicacid, N-acetyl-L-histidine, N-acetyl-L-isoleucine, N-acetyl-L-leucine, N-acetyl-L-lysine, N-acetyl-Lmethionine, N-acetyl-L-phenylalamine, N-acetyl-L-proline, N-acetyl-L-serine, N-acetyl-L-threonine, N-acetyl-L-tryptophan, N-acetyl-L-tyrosine, N-acetyl-L-valine, N-acetyl-D-alanine, N-acetyl-D-arginine, N-acetyl-D-asparagine, N-acetyl-D-aspartic acid, N-acetyl-D-cysteine, N-acetyl-D-glutamine, N-acetyl-D-glutamic acid, N-acetyl-D-histidine, N-acetyl-D-isoleucine, N-acetyl-D-leucine, N-acetyl-D-lysine, N-acetyl-D-methionine, N-acetyl-D-phenylalamine, N-acetyl-D-proline, N-acetyl-D-serine, N-acetyl- D-threonine, N-acetyl-D-tryptophan, N-acetyl-D-tyrosine or N-acetyl-D-valine.
An INDEPENDENT CLAIM is also included for the preparation of (I).
USE - (I) are useful as building blocks in the synthesis of optically active beta -amino acids and pharmaceutical drugs, via the resolution of racemic beta -amino alkylnitriles using, as resolving agents, optically active N-acetyl-alpha-amino adds.
ADVANTAGE - (I) provides a high yielding resolution reaction with very high selectivity and low cost/high efficiency procedure for synthesizing R-3-aminopentanenitrile.
Dwg.0/0
FS CPI
FA AB; GI; DCN
MC CPI: B06-D01; B07-D03; B07-D09; B10-A15

L41 ANSWER 2 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2005-180423 [19] WPIX
CR 2004-120526 [12]
DNC C2005-057788
TI Preparation of 3-amino nitrile compounds useful as intermediates for producing fine chemicals involves resolving mixture comprising two enantiomers of 3-aminopentane nitrile in presence of chiral acid in solvent system.
DC B05
IN ACHENBACH-MCCARTHY, C A; ALLEN, D R
PA (ACHE-I) ACHENBACH-MCCARTHY C A; (ALLE-I) ALLEN D R
CYC 1
PI US 2005038281 A1 20050217 (200519)* 9 C07C253-32
ADT US 2005038281 A1 Cont of US 2002-185092 20020628, US 2004-946167 20040921
PRAI US 2002-185092 20020628; US 2004-946167 20040921

IC ICM C07C253-32
AB US2005038281 A UPAB: 20050321
NOVELTY - Preparation of 3-amino nitrile compounds involves resolving enantiomeric mixture of (S)-3-aminopentane nitrile and (R)-3-aminopentane nitrile in presence of chiral acid (A1) in a solvent system to produce a chiral 3-amino nitrile salt.
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for new (R)-3-aminopentanenitrile dibenzoyl-(L)/(D)-tartrate salts.
USE - For the preparation of chiral amino-nitriles (claimed), useful as starting material for the production of fine chemicals.
ADVANTAGE - The chiral 3-amino nitrile salt has an optical purity of at least 45% (preferably 65 - 95%) e.e and the enantiomerically enriched 3-amino nitrile salt has an optical purity of at least 89% e.e.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B10-A15; B10-C02

L41 ANSWER 3 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-487170 [46] WPIX
DNC C2004-181421
TI Preparation of enantiomerically enriched 3-aminopentanenitriles to produce pharmaceutical products by reacting enantiomeric mixture containing R-3-aminopentanenitrile and S-3-aminopentanenitrile with an acyl donor in the presence of enzyme.
DC B05 D16 E16
IN ALLEN, D R; MOZHAEV, V V; VALIVETY, R H
PA (ALLE-I) ALLEN D R; (MOZH-I) MOZHAEV V V; (VALI-I) VALIVETY R H; (PCBU-N) PCBU SERVICES INC
CYC 106
PI US 2004121435 A1 20040624 (200446)* 12 C12P013-00
WO 2004058701 A2 20040715 (200446) EN C07D000-00
RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NI NO NZ OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW
AU 2003297360 A1 20040722 (200476) C12P013-00
ADT US 2004121435 A1 US 2002-327492 20021220; WO 2004058701 A2 WO 2003-US40508 20031219; AU 2003297360 A1 AU 2003-297360 20031219
FDT AU 2003297360 A1 Based on WO 2004058701
PRAI US 2002-327492 20021220
IC ICM C07D000-00; C12P013-00
AB US2004121435 A UPAB: 20040720
NOVELTY - Preparing (P1) enantiomerically enriched 3-aminopentanenitriles, comprising reacting an enantiomeric mixture (m1) containing R-3-aminopentanenitrile (R-APN) and S-3-aminopentanenitrile (S-APN) with an acyl donor in the presence of an enzyme to selectively acylate one of R-APN and S-APN, is new.
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for preparation (P2) of enantiomerically enriched 3-aminopentanenitriles, comprising selective hydrolyzing one of acylated R-APN and acylated S-APN present in an enantiomeric mixture (m2) containing acylated R-APN and acylated S-APN in the presence of an enzyme.
USE - For preparation of enantiomerically enriched 3-aminopentanenitriles useful to produce pharmaceutical products.
ADVANTAGE - The method is efficient, economic and is a convenient alternative for the chiral resolution of aminopentanenitriles. The biocatalyst used exhibit excellent enantioselectivities. The enzyme reactions are specific with mild reaction conditions.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B10-A15; D05-A02C; D05-C; E10-A15E

L41 ANSWER 4 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-464563 [44] WPIX
DNC C2004-173877
TI Manufacture of racemic amino pentane nitrile used for producing optically active amino pentane nitrile, involves racemizing optically active amino pentane nitrile by heating in presence of base and in atmosphere free of hydrogen.
DC B05 E16
PA (TORA) TORAY IND INC
CYC 1
PI JP 2004175741 A 20040624 (200444)* 7 C07C253-30
ADT JP 2004175741 A JP 2002-345094 20021128
PRAI JP 2002-345094 20021128
IC ICM C07C253-30
ICS C07C255-24
AB JP2004175741 A UPAB: 20040712
NOVELTY - An optically active amino pentane nitrile is racemized by heating in presence of a base and in an atmosphere free from hydrogen, to obtain racemic amino pentane nitrile.
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for manufacture of optically active amino pentane nitrile. A raw material containing racemic amino pentane nitrile is optically resolved, and one optically active amino pentane nitrile is separated, by optical resolution process. The remaining optically active amino pentane nitrile is racemized by racemization process, to obtain racemic amino pentane nitrile. Subsequently, the racemic amino pentane nitrile is recycled as raw material of optical resolution process, by recycle process. The optically active amino pentane nitrile is racemized by heating in presence of base and in atmosphere free of hydrogen, in racemization process.
USE - For manufacture of racemic amino pentane nitrile reused as raw material for optically active amino pentane nitrile manufacture (claimed) used as medicinal raw material.
ADVANTAGE - The unwanted optical isomers recovered by optical resolution of racemic amino pentane nitrile can be racemized easily. The racemic amino pentane nitrile obtained by the manufacturing method, can be effectively reused as raw material for optically active amino pentane nitrile manufacture.
Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B10-A15; E10-A15E

L41 ANSWER 5 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-395892 [37] WPIX
DNC C2004-148555
TI Production of optically active aminopentane nitrile such as optically active 3-aminopentane nitrile, by mixing optically active carboxylic acid with racemic aminopentane nitrile and optically resolving obtained diastereomeric salt.
DC B05
PA (TORA) TORAY IND INC
CYC 1
PI JP 2004143108 A 20040520 (200437)* 7 C07C253-34
ADT JP 2004143108 A JP 2002-311182 20021025
PRAI JP 2002-311182 20021025
IC ICM C07C253-34
ICS C07C255-24
AB JP2004143108 A UPAB: 20040611
NOVELTY - Production of optically active aminopentane nitrile involves mixing optically active carboxylic acid with racemic aminopentane nitrile in a solvent and optically resolving the obtained diastereomeric salt.
USE - Used for production of optically active aminopentane nitrile such as optically active 3-aminopentane nitrile (claimed) useful as medicinal raw material.
ADVANTAGE - The method is convenient and cost effective.

Dwg.0/0
FS CPI
FA AB; DCN
MC CPI: B10-A15

L41 ANSWER 6 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-122968 [12] WPIX
DNC C2004-049612
TI Producing optically-active beta-amino compounds and antipode amide compounds for use in pharmaceutical and agrochemical intermediates, comprises asymmetric enzymatic hydrolysis with stereoselectivity.
DC B05 C03 D16
IN ITO, N; KAWANO, S; YASOHARA, Y
PA (KANF) KANEKA CORP
CYC 105
PI WO 2004007741 A1 20040122 (200412)* JA 32 C12P041-00
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NI NO NZ OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW
AU 2003280995 A1 20040202 (200450) C12P041-00
ADT WO 2004007741 A1 WO 2003-JP8826 20030711; AU 2003280995 A1 AU 2003-280995 20030711
FDT AU 2003280995 A1 Based on WO 2004007741
PRAI JP 2003-47363 20030225; JP 2002-204592 20020712
IC ICM C12P041-00
ICS C07C255-29
ICA C12R001-05
ICI C12R001:15, C12R001:365, C12R001:72
AB WO2004007741 A UPAB: 20040218
NOVELTY - Producing an optically-active beta -amino compound (II) and its antipode amide compound comprising acting on an amide compound (I) with an enzyme source having asymmetric hydrolysis activity, is new.
DETAILED DESCRIPTION - Producing an optically-active beta - amino compound of formula (II) and its antipode amide compound comprises acting on an amide compound of formula (I) with an enzyme source having asymmetric hydrolysis activity.
formula (I)
R1 = 1-8C alkyl, 1-8C alkoxy, 2-8C alkenyl or 2-8C alkynyl
R2 = 1-8C alkyl, 1-8C alkoxy, 2-8C alkenyl, 2-8C alkynyl, 6-14C aryl or 5-14C heterocyclyl.
formula (II)
asterisk = asymmetric carbon atom.
INDEPENDENT CLAIMS are also included for:
(1) an amide compound of (III) or its salt; and
(2) an optically-active isomer of the amide compound of formula (III).
R3 = 1-8C alkyl, 1-8C alkoxy, 2-8C alkenyl or 2-8C alkynyl
R4 = 1-8C alkyl, 1-8C alkoxy, 2-8C alkenyl, 2-8C alkynyl, 6-14C aryl or 5-14C heterocyclyl.
USE - The produced compounds are for use, e.g. in pharmaceutical and agrochemical intermediates.
ADVANTAGE - Such efficient method has high stereoselectivity.
Dwg.0/0
FS CPI
FA AB; GI; DCN
MC CPI: B10-A15; C10-A15; D05-A02C; D05-A04

L41 ANSWER 7 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-120526 [12] WPIX
CR 2005-180423 [19]
DNC C2004-048500
TI Preparation of 3-amino nitrile compounds useful as intermediates for the

production of fine chemicals involves resolving chiral 3-amino nitrites in presence of chiral acid in a solvent to produce a chiral 3-amino nitrile salt.

DC B05

IN ACHENBACH-MCCARTHY, C; ALLEN, D R; ACHENBACH-MCCARTHY, C A

PA (PCBU-N) PCBU SERVICES INC; (ACHE-I) ACHENBACH-MCCARTHY C A; (ALLE-I) ALLEN D R

CYC 103

PI US 2004002615 A1 20040101 (200412)* 9 C07C253-32
WO 2004002924 A1 20040108 (200413) EN C07B057-00
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT RO RU SC SD SE SG SK SL TJ TM TN TR TT TZ UA UG UZ VC VN YU ZA ZM ZW
AU 2003245572 A1 20040119 (200447) C07B057-00
EP 1517877 A1 20050330 (200522) EN C07B057-00
R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV MC MK NL PT RO SE SI SK TR
KR 2005016625 A 20050221 (200542) C07C253-32

ADT US 2004002615 A1 US 2002-185092 20020628; WO 2004002924 A1 WO 2003-US19271 20030619; AU 2003245572 A1 AU 2003-245572 20030619; EP 1517877 A1 EP 2003-739199 20030619, WO 2003-US19271 20030619; KR 2005016625 A KR 2004-720987 20041223

FDT AU 2003245572 A1 Based on WO 2004002924; EP 1517877 A1 Based on WO 2004002924

PRAI US 2002-185092 20020628

IC ICM C07B057-00; C07C253-32
ICS C07C253-30; C07C255-24

AB US2004002615 A UPAB: 20050704
NOVELTY - Preparation of 3-amino nitrile compounds involves resolving an enantiomeric mixture of chiral 3-amino nitrites in the presence of a chiral acid in a solvent (S1) to produce a chiral 3-amino nitrile salt (I).
USE - For preparing 3-amino nitrile compounds e.g. (R) and (S) 3-aminopentanenitrile (claimed), useful as intermediates for the production of fine chemicals.
ADVANTAGE - (I) Has an optical purity of (at least 45, preferably 65 - 95)% ee. The enantiomerically enriched (I) has an optical purity of at least 89% ee. The method involves a single step and has improved yields compared to the prior art multi-step processes.
Dwg.0/0

FS CPI

FA AB; DCN

MC CPI: B10-A15; B10-C02; **B11-B**

L41 ANSWER 8 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2003-512515 [48] WPIX

DNC C2003-137248

TI Preparation of chiral amino nitrile compounds used as starting material in synthesis of fine chemicals comprises esterifying amino protected alcohol, followed by nucleophilic substitution of ester with cyano.

DC B05 E16

IN ACHENBACH-MCCARTHY, C A; ALLEN, D R

PA (ACHE-I) ACHENBACH-MCCARTHY C A; (ALLE-I) ALLEN D R; (PCBU-N) PCBU SERVICES INC

CYC 102

PI US 2003065207 A1 20030403 (200348)* 12 C07C253-16
WO 2003029190 A1 20030410 (200348) EN C07C253-16
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SK SL SZ TR TZ UG ZM ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT

RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG UZ VC VN YU ZA ZM ZW
US 6610874 B2 20030826 (200357) C07C253-16
EP 1430021 A1 20040623 (200441) EN C07C253-16
R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI SK TR
AU 2002337723 A1 20030414 (200461) C07C253-16
KR 2004047870 A 20040605 (200465) C07C253-16
JP 2005504825 W 20050217 (200513) 36 C07C269-06
ADT US 2003065207 A1 US 2001-967270 20010928; WO 2003029190 A1 WO 2002-US30728 20020927; US 6610874 B2 US 2001-967270 20010928; EP 1430021 A1 EP 2002-773615 20020927, WO 2002-US30728 20020927; AU 2002337723 A1 AU 2002-337723 20020927; KR 2004047870 A KR 2004-704537 20040326; JP 2005504825 W WO 2002-US30728 20020927, JP 2003-532444 20020927
FDT EP 1430021 A1 Based on WO 2003029190; AU 2002337723 A1 Based on WO 2003029190; JP 2005504825 W Based on WO 2003029190
PRAI US 2001-967270 20010928
IC ICM C07C253-16; C07C269-06
ICS C07B053-00; C07C253-30; C07C255-24; C07C255-30; C07C271-20
AB US2003065207 A UPAB: 20030729
NOVELTY - Preparation of chiral amino nitrile compounds (I) comprises:
(a) esterifying the alcohol group of a chiral amino alcohol having an alcohol group and a protected amine group to form an electrophilic carbon having a leaving group, and
(b) substituting a cyanide for the leaving group in the presence of dimethylformamide to form chiral amino nitrile having a protected amine group.
USE - Used for the preparation of (I), preferably N-t-butoxycarbonyl-(3R)-aminopentanenitrile (Ia) and (3R)-aminopentanenitrile (claimed) useful as intermediates in the synthesis of cholesterol reducing agent, and as starting materials and intermediates in the synthesis of fine chemicals.
ADVANTAGE - The process is efficient and gives high yields of (I) while using inexpensive reagents. The amino alcohol used in the process is industrially feasible.
Dwg.0/6
FS CPI
FA AB; GI; DCN
MC CPI: B10-A15; E10-A15E; E11-H

L41 ANSWER 9 OF 9 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1999-312238 [26] WPIX
DNC C1999-092129
TI Cyanobutylation of ammonia, alkylamines and hydrazine with 3- and 4-pentenenitriles to form alkylaminonitriles.
DC A21 A41 A60 E13 E16
IN HERKES, F E
PA (DUPO) DU PONT DE NEMOURS & CO E I
CYC 1
PI US 5902883 A 19990511 (199926)* 4 C07D241-04
ADT US 5902883 A US 1997-993967 19971218
PRAI US 1997-993967 19971218
IC ICM C07D241-04
ICS C07C255-00
AB US 5902883 A UPAB: 20011211
NOVELTY - Cyclobutylation of ammonia, primary and secondary alklamines and hydrazine with 3- and/or 4-pentenenitriles to form alkylaminonitriles
DETAILED DESCRIPTION - A process for making aliphatic 3-aminonitriles comprises:
(i) forming a reaction mixture comprising 3- and/or 4-pentenenitrile and ammonia or an alkamine; or
(ii) optionally incorporating water into the reaction mixture; and
(iii) reacting the mixture at 25-200 deg. C and pressures from autogeneous to 1500 psig.
USE - The process is used for the cyanobutylation of ammonia, alkylamines and hydrazine with 3- and 4-pentenenitriles to form

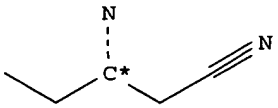
alkylaminonitriles which can be hydrogenated to form alkyldiamines. The alkyldiamines can be used as monomers for producing polyamide, polyimide or polyurethane urea. The alkyldiamines can also be used as a metal chelating agent or an epoxy resin crosslinker.

ADVANTAGE - Alkylaminonitriles can be made with high yields and selectivity's. The reaction rate is increased by the addition of a strong base

FS CPI
FA AB; GI; DCN
MC CPI: A01-E05; A05-A01B1; A08-D03; E07-D11; E10-A15D; E10-A15E; E10-B01E; E31-A04

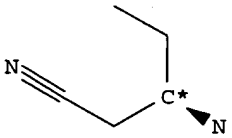
=> d std l31 tot

L31 ANSWER 1 OF 3 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN.S **DCR-923913**
DCSE 211181-4-0-0
CN.S 3-Amino-pentanenitrile



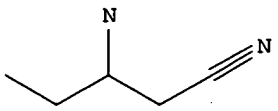
MF **C5 H10 N2**

L31 ANSWER 2 OF 3 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN.S **DCR-738940**
DCSE 211181-1-0-0
CN.S 3-Amino-pentanenitrile



MF **C5 H10 N2**

L31 ANSWER 3 OF 3 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN.S **DCR-211181**
DCSE 211181-0-0-0
CN.S 3-Amino-pentanenitrile



MF **C5 H10 N2**

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